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About New Methods in the Theory of Superconductivity

III

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In the past great success was attained in solution of statistical physics problems using the method of summation of most important graphs.

In present article we will show, that in the theory of superconductivity it is possible to obtain by this method the same results, that were found in previous works (1, 2) with the aid of canonic transformation and principle of compensation of graphs with a "dangerous" energy denominator.

As was shown by V. V. Tolmachev and S. V. Tiablikov, to consider the Bardeen's Hamiltonian instead it is possible of Fröhlich's Hamiltonian, for they both are actually completely equivalent in accounting the influence of electron-phonon interaction on the electron dynamics near the Fermi surface. In this case it is much simpler to use Bardeen's Hamiltonian.

Therefore, for the sake of illustration and establishment of connection with the ideas presented in the work of Bardeen, Cooper and Schrieffer (3), we shall proceed from Bardeen's Hamiltonian:

$$H_B = \sum_{\mathbf{k}s} E(\mathbf{k}) a_{\mathbf{k}s}^+ a_{\mathbf{k}s}$$

$$- \frac{Y}{V} \sum_{(k_1, k_2, k'_1, k'_2)} a_{k_1, -2}^+ a_{k_2, 2}^+ a_{k'_1, 2} a_{k'_2, -2} \Theta(k_1) \Theta(k'_1) \Theta(k'_2) \Delta(k_1 + k_2 - k'_1 - k'_2)$$

where

$$\Theta(k) = \begin{cases} 1, & E(k_F) - \omega < E(k) < E(k_F) + \omega \\ 0, & |E(k) - E(k_F)| > \omega \end{cases}$$

$$\Delta(k) = \begin{cases} 1, & k = 0 \\ 0, & k \neq 0 \end{cases}$$

and where $E(\mathbf{k})$ is a radially-symmetrical function representing the energy of an electron with impulse \mathbf{k} ,

γ & η are the Bardeen's parameters.

In Fröhlich's model we should set ⁽²⁾.

$$\gamma = g^2, \quad \omega = \frac{\tilde{\omega}}{2}$$

We will account the quantity N of whole number of electrons with the aid of chemical potential λ . For this we add $-\lambda_N$ to H_0

Hence we get Hamiltonian

$$H = H_0 + H_{int}$$

$$H_0 = \sum_{\mathbf{k}, s} \{E(\mathbf{k}) - \lambda\} a_{\mathbf{k}s}^+ a_{\mathbf{k}s} \quad (1)$$

$H_{int} =$

$$= \frac{Y}{V} \sum a_{\mathbf{k}_1, \downarrow}^+ a_{\mathbf{k}_2, \downarrow}^+ a_{\mathbf{k}_2', \uparrow} a_{\mathbf{k}_1', \uparrow} \Theta(\mathbf{k}_1) \Theta(\mathbf{k}_2) \Theta(\mathbf{k}_1') \Theta(\mathbf{k}_2') \Delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_1' - \mathbf{k}_2')$$

for which we shall consider the question about the summation of the most important graphs. In so far as the interaction is effective only in a small region of Fermi surface and only between the particles (electrons or holes) with oppositely oriented spins, we see that the graphs of the type illustrated in Fig. 1 will play an especially important role. These graphs were constructed from "indivisible complex" (see Fig. 2)



Fig. 1

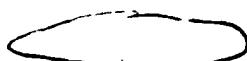


Fig. 2

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consisting of a pair of particles with impulse $\pm \mathbf{k}$ and spins $\pm \frac{1}{2}$. For their summation we will use the method of approximate secondary quantization i.e. we will construct a simplified Hamiltonian which will have graphs only of that class which we wish to sum up, but with the same contribution as in real Hamiltonian.

In so far as in the presently examined graphs the groups of the particle pair $(\pm \mathbf{k}, \pm \frac{1}{2})$ do not break, it is natural to compare them with the quantum amplitudes $b_{\mathbf{k}}$, $b_{\mathbf{k}}^+$ with commutation relations:

$$[b_{\mathbf{k}}, b_{\mathbf{k}'}] = 0, [b_{\mathbf{k}}^+, b_{\mathbf{k}'}^+] = 0, [b_{\mathbf{k}}^+, b_{\mathbf{k}'}] = 0; \mathbf{k} + \mathbf{k}' \quad (2)$$

Further, because several pairs with the same value of \mathbf{k} do not exist, we must let

$$b_{\mathbf{k}}^2 = 0 \quad (3)$$

We should also note, that the group's self energy will be $2\{E(\mathbf{k}) - \lambda\} b_{\mathbf{k}}^+ b_{\mathbf{k}}$

and that the matrix element of Hamiltonian (1) for transition will be proportional $- \frac{y}{V}$.

From these considerations we get the simplified Hamiltonian in form

$$H = H_0 + H_{int}$$

$$H_0 = \sum_{\mathbf{k}} 2\{E(\mathbf{k}) - \lambda\} b_{\mathbf{k}}^+ b_{\mathbf{k}} \quad (4)$$

$$H_{int} = - \frac{y}{V} \sum_{\mathbf{k} + \mathbf{k}'} b_{\mathbf{k}}^+ b_{\mathbf{k}'}^+ \Theta(\mathbf{k}) \Theta(\mathbf{k}')$$

containing the operators b_k , b_k^* . ^{writ} Let us call these operators the Pauli-operators. Let us take

an expression of any order

$$H_{int} (H_0 - E)^{-1} H_{int} (\mu_0 - E)^{-1} H_{int}$$

now, it is easy to verify directly that, the sum of contributions from the graphs of the type being examined for the Hamiltonian (I) will be equal to the sum of contributions of all the graphs for the simplified Hamiltonian (4). Hence the problem of summation of the special class of graphs for Hamiltonian (I) turns out to be equivalent to the problem of dynamic system model, characterized by Hamiltonian (4).

We start the construction of asymptotically exact solution of this latter problem, neglecting only those values that disappear in the process of the limiting transition $V \rightarrow \infty$. We shall distinguish the electron pairs from hole pairs. Therefore, we introduce new Pauli-operators by letting

$$\beta_k = b_k \quad ; \quad E(k) > \lambda$$

$$\beta_k^* = b_k^* \quad ; \quad E(k) < \lambda$$

We get

$$H = U + 2 \sum_k |E(k) - \lambda| \beta_k^* \beta_k - \\ - \frac{1}{V} \sum_{kk'} \Theta(k) \Theta(k') \{ \theta_F(k) \beta_k^* + \theta_G(k) \beta_k \} \{ \theta_G(k') \beta_{k'} + \theta_F(k') \beta_{k'}^* \} \quad (5)$$

where

$$\theta_F(k) + \theta_G(k) = 1$$

$$\theta_F(k) = \begin{cases} 1, & E(k) < \lambda \\ 0, & E(k) > \lambda \end{cases}$$

$$U = 2 \sum_k \{E(k) - \lambda\} \theta_F(k)$$

Let's consider
the number of
numbers in \mathcal{C} .

$$\mathcal{C} \subset \mathbb{C}^V$$

Let $\mathcal{C}_k = \{c_k\}$ be the set of vectors in \mathcal{C} with $c_k \neq 0$.

exact application of the theorem.

Indeed we have

$$H = H' + H'' + U$$

$$\begin{aligned} H' &= 2 \sum_k |E(k) - \lambda| \beta_k^\dagger \beta_k - \\ &\quad - \frac{1}{V} \sum_{K \neq k'} \Theta(K) \Theta(K') \{ \Theta_G(k) \beta_k^\dagger + \Theta_F(k) \beta_k \} \Theta_G(k') \beta_{k'} - \\ &\quad - \frac{1}{V} \sum_{K \neq k'} \Theta(k) \Theta(k') \Theta_F(k) \Theta_F(k') \beta_k^\dagger \beta_{k'} \\ H'' &= - \frac{1}{V} \sum_{K \neq k'} \Theta(k) \Theta(k') \Theta_F(k) \Theta_F(k') \beta_k^\dagger \beta_{k'} \end{aligned}$$

But obviously

$$H \subset \mathcal{C}$$

On the other hand

$$\langle C^* | H'' |^2 C \rangle = \langle C^* H''^\dagger H'' C \rangle$$

$$= \frac{1}{V^2} \sum_{K \neq k'} \Theta(k) \Theta(k') \Theta_F(k) \Theta_F(k') \subset \text{const}$$

$$V \rightarrow \infty$$

But in the process of filling the shell the number of electrons will remain finite. Therefore the average occupation number remains finite. Furthermore, since the occupation number is a proper function of a given electron configuration we have

$$\bar{N} = \langle C^* N_C \rangle = \sum z$$

By equating this expression to the whole number of electrons in the Fermi shell

$$\sum z \\ \text{we see, that } E_F = E(K_F)$$

Now, let us analyze the question of stability of condition 3

Let us examine first the case when

$$\gamma < 0$$

To the double sum of (1) we add the members for which $\lambda > K_F$. Doing this we do not introduce any quantities that would contribute in transition to the limit $V \rightarrow \infty$. We note then, that $H-U$ is essentially equal to the positive form. The value of U , consequently, will be minimum, and therefore the state C will be stable. A different situation will be in the case

$$\gamma > 0$$

Note, that in this case in state C all occupation numbers $n_{\alpha}, \beta_{\alpha}, \beta^*$ are equal to zero; and in calculation of elementary excitation energy we can regard the Pauli-like operators β, β^* as Bose-operators. It only remains that to diagonalize the quadratic form from operators β, β^* representing $H-U$ (5). This diagonalization can be done, for example with the aid

of the potential energy

For definiteness we consider the case of a rectangular cavity

so we get the following equation

$$I = \frac{Y}{V} \sum_k E_k \left\{ \frac{\partial^2 U}{\partial x_k^2} + \frac{\partial^2 U}{\partial y_k^2} \right\}$$

$E_k = 2 \pi E_F k_x k_y$,
from where we find after simplification

$$I = \frac{Y}{V} \sum_{E_F < E(k_x, k_y)} \frac{2 E_k}{E_k - E}^2$$

or

$$I = \frac{\rho}{2} \int_0^\infty K^2 \frac{dK}{dE} \frac{2Z dz}{Z^2 - E^2}$$

(1)

where

$$\rho = \frac{Y}{(2\pi)^2} \left(\frac{K^2 f_K}{f_E} \right)$$

As is evident, this equation in the case under examination (1) always has negative roots for E . Consequently, we get purely imaginary values for the energy E

$$E \sim i \omega e^{-\frac{1}{\rho}}$$

Hence, the stable condition (10) is equivalent to the condition that the amplitudes β_k, β_k^+ satisfy the equations (11), but with α and β replaced by

$$\beta_k = U_k V_k (2b_k^+ b_k - 1) + U_k^2 b_k - V_k^2 \alpha_k^+$$

$$\beta_k^+ = U_k V_k (2b_k^+ b_k - 1) - V_k^2 b_k + U_k b_k^+$$

where U_k, V_k - are real numbers, bound by equality

$$U_k^2 + V_k^2 = 1$$

It is easy to observe, that amplitudes of (11) really satisfy all commutation relations of the \hat{a} -operator.

Reducing the transformation (10), we find

$$b_k = U_k V_k (-2\beta_k^+ \beta_k) + U_k^2 \beta_k - V_k^2 \alpha_k^+$$

$$b_k^+ = U_k V_k (1 - 2\beta_k^+ \beta_k) - V_k^2 \beta_k + U_k^2 \beta_k^+$$

$$b_k^+ b_k = V_k^2 + (U_k^2 - V_k^2) \beta_k^+ \beta_k + U_k V_k (\beta_k + \beta_k^+) \quad (12)$$

Substituting these expressions into hamiltonian (4), we find

$$\begin{aligned} H = & U + \sum_k \left\{ 2(E(k) - \lambda) U_k V_k - \right. \\ & - \frac{y}{V} \Theta(k) (U_k^2 - V_k^2) \sum_{k'} \Theta(k') [i, U_{k'}] \left. \right\} (\beta_k + \beta_k^+) \quad (13) \\ & + \sum_k 2E(k) \beta_k^+ \beta_k - \\ & - \frac{y}{V} \sum_{k_1+k_2} \left\{ U_{k_1}^2 \beta_{k_1}^+ - b_{k_1}^+ b_{k_1} - 2U_{k_1} V_{k_1} \beta_{k_1}^+ \beta_{k_1} \right\} \\ & \times \left\{ U_{k_2}^2 \beta_{k_2} - b_{k_2}^+ b_{k_2} - 2U_{k_2} V_{k_2} \beta_{k_2}^+ \beta_{k_2} \right\} C(k) \Theta(k_2) \end{aligned}$$

where $U = \sum_k \{E(k) - \lambda\} U_k^2 - \frac{3}{V} \sum_{k_1, k_2} S(k_1, k_2) U_{k_1} U_{k_2}$ (14)

$$E_e(k) = E(k) + \lambda + \frac{2}{V} \sum_{k'} S(k') U_{k'}$$
 (15)

In the expression (15) all the coefficients of $\beta_{k'} - \beta_k$ equal to zero. We get then the equation

$$2(E(k) - \lambda) U_k V_k - \frac{3}{V} \Theta(k) (U_k^2 - V_k^2) \sum_{k'} S(k') U_{k'} V_{k'} = 0 \quad (16)$$

found in work by (2) with the aid of dangerous graph compensation principle. Noticing that with required here exactness $\lambda = E(k_F)$ we get same as in (2)

$$U^2(k) = \frac{1}{2} \left\{ 1 + \frac{E(k) - E(k_F)}{\sqrt{(E(k) - E(k_F))^2 + \Theta(k)} C^2} \right\}$$

$$V^2(k) = \frac{1}{2} \left\{ 1 + \frac{E(k_F) - E(k)}{\sqrt{(E(k) - E(k_F))^2 + \Theta(k)} C^2} \right\}$$

$$C = 2\omega e^{-\frac{k}{\lambda}} \quad (17)$$

$$E_e(k) = \sqrt{(E(k) - E(k_F))^2 + \Theta(k) C^2}$$

Hamiltonian (15) now can be presented in form of

$$H = H_0 + H' + H'' + U$$

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where $H_0 = \sum_k 2E_k / V_k \rho_{kk}$

$$H' = -\frac{y}{V} \sum_{k_1 \neq k_2} \Theta(k_1) \Theta(k_2) \{ U_{k_1}^2 \beta_{k_1}^+ - V_{k_1}^2 \beta_{k_1} \} \{ U_{k_2}^2 \beta_{k_2} - V_{k_2}^2 \beta_{k_2}^+ \}$$

$$\begin{aligned} H'' &= 2 \frac{y}{V} \sum_{k_1 \neq k_2} \Theta(k_1) \Theta(k_2) \{ U_{k_2}^2 \beta_{k_2} - V_{k_2}^2 \beta_{k_2}^+ - 2 U_{k_2} V_{k_2} \beta_{k_2}^+ \beta_{k_1} \} U_{k_1} V_{k_1} \beta_{k_1}^+ \beta_{k_1} + \\ &+ 2 \frac{y}{V} \sum_{(k_1 \neq k_2)} \Theta(k_1) \Theta(k_2) \{ U_{k_1}^2 \beta_{k_1}^+ - V_{k_1}^2 \beta_{k_1} - 2 U_{k_1} V_{k_1} \beta_{k_1}^+ \beta_{k_2} \} U_{k_2} V_{k_2} \beta_{k_2}^+ \beta_{k_1} \end{aligned} \quad (18)$$

Let us take the wave function C , for which all occupation numbers

$$V_k = \beta_k^+ \beta_k$$

are equal to zero. We will show, as previously, that with accuracy up to the values disappearing in the process of limiting transition $V \rightarrow \infty$, C is a proper function of Hamiltonian H , giving it a value of U . We have, really,

$$(H_0 + H'')C = 0$$

and

$$\langle C^* | H'' |^2 C \rangle = \frac{y^2}{V^2} \sum_{k_1 k_2} \Theta(k_1) \Theta(k_2) \{ U_{k_1}^4 V_{k_2}^4 + U_{k_1}^2 V_{k_1}^2 U_{k_2}^2 V_{k_2}^2 \} \underset{V \rightarrow \infty}{\text{const}}$$

Now let us examine elementary excitations. Because in state C all occupation numbers V_k are equal to zero, in calculation of elementary excitation energy we can regard the Pauli-operators β_k, β_k^+ as Bose-operators and in hamiltonian expression (18) we can restrict ourselves to quadratic form $H_0 + H'$

Diagonalizing it by the method mentioned previously (4) we are getting to the solution of the equation

$$\begin{aligned}
 (\epsilon - 2E_e(k))\phi_k &= \Theta(k) U_k \frac{Y}{V} \sum_k \{U_k^2 \phi_k - V_k^2 \chi_k\} S(k) - \\
 &\quad - \Theta(k) V_k \frac{Y}{V} \sum_k \{U_k^2 \chi_k - V_k^2 \phi_k\} B(k) \\
 - (\epsilon + 2E_e(k))\chi_k &= B(k) U_k^2 \frac{Y}{V} \sum_k \{U_k^2 \chi_k - V_k^2 \phi_k\} S(k) \\
 &\quad - \Theta(k) V_k^2 \frac{Y}{V} \sum_k \{U_k^2 \phi_k - V_k^2 \chi_k\} B(k)
 \end{aligned} \tag{19}$$

with normalizing condition

$$\sum_k \{|\phi_k|^2 - |\chi_k|^2\} = 1 \tag{20}$$

From here we get secular equation

$$\begin{aligned}
 &\left\{ 1 + \frac{Y}{V} \sum_k \Theta(k) \left[\frac{U_k^4}{2E_e(k)+\epsilon} + \frac{V_k^4}{2E_e(k)-\epsilon} \right] \right\} \times \\
 &\times \left\{ 1 + \frac{Y}{V} \sum_k \Theta(k) \left[\frac{V_k^4}{2E_e(k)+\epsilon} + \frac{U_k^4}{2E_e(k)-\epsilon} \right] \right\} \\
 &- \left\{ \frac{Y}{V} \sum_k \Theta(k) U_k^2 V_k^2 \left[\frac{1}{2E_e(k)+\epsilon} + \frac{1}{2E_e(k)-\epsilon} \right] \right\}^2
 \end{aligned} \tag{21}$$

It is not difficult to notice, that when

$$|\epsilon| < 2_{\min} E_e(k) = 2E_e(k_F)$$

this equation has no solutions, for the subtrahend in (21) is smaller than minuend. In case

$$|\epsilon| > 2E_e(k_F)$$

there is a continuous spectrum

$$E = \pm 2E_e(k) + O\left(\frac{1}{v}\right)$$

$$O\left(\frac{1}{v}\right) \rightarrow 0 \quad \text{when} \quad v \rightarrow 0$$

as can be seen from (19) - sign does not agree with the normalizing condition (20).

Hence, all E's are positive (this could be foreseen by noticing directly that the quadratic form under examination is definitely positive) and are separated from zero by a gap

$$E = 2E_e(k) \gg 2E_e(k_F) = 2c = 4\omega e^{-\frac{1}{\theta}} \quad (2c)$$

Here again we get the same Bardeen's results, as in previous works (1, 2). As we can see, the graph summation method appears to be quite descriptive and it does permit the establishment of connection with the ideas presented in the work of Bardeen-Cooper-Schrieffer.

Nevertheless, in our opinion, the method of canonic transformation is more flexible and permits to obtain higher approximations quite easily. Besides it permits various generalizations; for example, in calculation of thermodynamic quantities.

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